

CBE 633: Multiscale Materials Modeling
Spring, 2012
Schedule

Meeting Place: Dougherty Engineering Building Room 314
Meeting Time: Fridays, 12:20-3:00

Lecture	Date	Topic
1	01/13/12	Introduction & Organization
2	01/20/12	Lecture 01. Capability of Quantum Mechanical Calculations (Keffer) Lecture 02. Capability of Classical Molecular Simulations (Keffer)
3	01/27/12	Lecture 03: Capability of Mesoscale Simulations (Keffer) Lecture 04: Capability of Continuum Simulations (Keffer)
4	02/03/12	Lecture 05: Example: Proton Transport (Keffer) Student 01 Background Presentation (Alex) Student 02 Background Presentation (DJ)
5	02/10/12	Lecture 06: Example: Polymers (Keffer) Student 03 Background Presentation (Carlos) Student 04 Background Presentation (Daniel) Student 05 Background Presentation (Sagar)
6	02/17/12	Student 06 Background Presentation (Marshall) Student 07 Background Presentation (Qianping) Student 08 Background Presentation (Nethika)
7	02/24/12	Lecture 07: Development of Coarse-Grained Potentials (Keffer)
8	03/02/12	Lecture 08: Pair Correlation Functions as Messengers (Keffer) Student 01 Progress Presentation (Alex) Student 02 Progress Presentation (DJ)
9	03/09/12	Student 03 Progress Presentation (Carlos) Student 04 Progress Presentation (Daniel) Student 05 Progress Presentation (Sagar)
10	03/16/12	Student 06 Progress Presentation (Marshall) Student 07 Progress Presentation (Qianping) Student 08 Progress Presentation (Nethika)
12	03/23/12	SPRING BREAK – NO CLASS
13	03/30/12	KEFFER OUT OF TOWN – NO CLASS
14	04/06/12	Lecture 09: Quantum Mechanics/Molecular Mechanics (Keffer) Lecture 10: Adaptive Resolution (Keffer)
15	04/13/12	Lecture 11: Linking with the Continuum Scale (Keffer) Student 01 Final Presentation (Alex) Student 02 Final Presentation (DJ)
16	04/20/12	Student 03 Final Presentation (Carlos) Student 04 Final Presentation (Daniel) Student 05 Final Presentation (Sagar)
17	04/27/12	Student 06 Final Presentation (Marshall) Student 07 Final Presentation (Qianping) Student 08 Final Presentation (Nethika)
18	05/04/12	Final Report due by noon.